

1H-Imidazole-5-sulfonic acid
60634-74-4 | DTXSID80524673

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.66e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.47e-01

Confidence level: 3.65e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chlorthion</div> <div>Measured: 2.00e-08</div> <div>Predicted: 6.17e-06</div>	<div>Image not found</div> <div>beta-Ionone</div> <div>Measured: 9.80e-08</div> <div>Predicted: 5.46e-02</div>	<div>Image not found</div> <div>Furalaxyl</div> <div>Measured: 1.13e-06</div> <div>Predicted: 3.22e-07</div>
<div>Image not found</div> <div>Dimercaprol</div> <div>Measured: 4.40e-07</div> <div>Predicted: 8.53e-03</div>		